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The Karlin–McGregor formula for a variant of a discrete version of Walsh's spider*

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Abstract

We consider a variant of a discrete space version of Walsh's spider, see Walsh (1978 *Temps Locaux, Asterisque* **vol 52–53** (Paris: Soc. Math. de France)) as well as Evans and Sowers (2003 *Ann. Probab.* **31** 486–527 and its references). This process can be seen as an instance of a quasi-birth-and-death process, a class of random walks for which the classical theory of Karlin and McGregor can be nicely adapted as in Dette, Reuther, Studden and Zygmunt (2006 *SIAM J. Matrix Anal. Appl.* **29** 117–42), Grünbaum (2007 *Probability, Geometry and Integrable Systems* ed Pinsky and Birnir **vol 55** (Berkeley, CA: MSRI publication) pp. 241–60, see also arXiv math PR/0703375), Grünbaum (2007 *Dagstuhl Seminar Proc. 07461 on Numerical Methods in Structured Markov Chains* ed Bini), Grünbaum (2008 *Proceedings of IWOTA*) and Grünbaum and de la Iglesia (2008 *SIAM J. Matrix Anal. Appl.* **30** 741–63). We give here a weight matrix that makes the corresponding matrix-valued orthogonal polynomials orthogonal to each other. We also determine the polynomials themselves and thus obtain all the ingredients to apply a matrix-valued version of the Karlin–McGregor formula.

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1. Birth-and-death processes and orthogonal polynomials

For the benefit of the reader we start with very classical material.

* Dedicated to Jack Schwartz, who passed away on March 2, 2009.

If $\mathbb{P}$ denotes the one-step transition probability matrix for a birth and death process on the non-negative integers

$$\mathbb{P} = \begin{pmatrix} r_0 & p_0 & 0 & 0 & \\ q_1 & r_1 & p_1 & 0 & \\ 0 & q_2 & r_2 & p_2 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

there is a powerful tool to analyze the random walk in question, [KMcG] as well as [vD, ILMV].

Introduce the polynomials $Q_j(x)$ by the conditions $Q_{-1}(0) = 0$, $Q_0(x) = 1$ and use the notation

$$Q(x) = \begin{pmatrix} Q_0(x) \\ Q_1(x) \\ \vdots \end{pmatrix}$$

to define the polynomials $Q_j(x)$ by the relation

$$\mathbb{P}Q(x) = xQ(x).$$

This definition is a compact way of writing down the three term recursion relation that defines the polynomials $Q_j(x)$.

One proves the existence of a unique orthogonality measure $\mathrm{d}\psi(x)$ supported in $[-1, 1]$ such that

$$\pi_j \int_{-1}^{1} Q_i(x) Q_j(x) \mathrm{d}\psi(x) = \delta_{ij}.$$

The same spectral theorem that is behind the expression above yields the Karlin–McGregor representation formula

$$(\mathbb{P}^n)_{ij} = \pi_j \int_{-1}^{1} x^n Q_i(x) Q_j(x) \mathrm{d}\psi(x).$$

Many probabilistic properties of the walk are reflected in the orthogonality measure that appears above. For instance the process is recurrent exactly when the integral

$$\int_{-1}^{1} \frac{\mathrm{d}\psi(x)}{1-x}$$

diverges. The process returns to the origin in a finite expected time when the measure has a mass at $x = 1$. The existence of

$$\lim_{n\to\infty} (\mathbb{P}^n)_{ij}$$

is equivalent to $\mathrm{d}\psi(x)$ having no mass at $x = -1$.

In some cases all the ingredients that go into this formula can be computed explicitly.

As an example suppose that we have $r_1 = r_2 = \cdots = 0, q_1 = q_2 = \cdots = q$ and $p_1 = p_2 = \cdots = p$, with $0 \leqslant p \leqslant 1$ and $q = 1 - p$.

One can show that

$$Q_j(x) = \left(\frac{q}{p}\right)^{j/2} [2(p_0 - p)/p_0 T_j(x^*) + (2p - p_0)/p_0 U_j(x^*) - r_0/p_0 (p/q)^{1/2} U_{j-1}(x^*)],$$

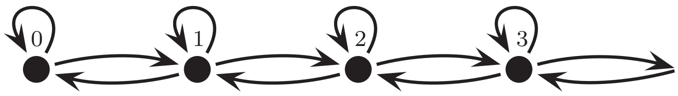
where T_j and U_j are the Chebyshev polynomials of the first and second kind, and $x^* = x/(2\sqrt{pq})$. The polynomials $Q_j(x)$ are orthogonal with respect to a spectral measure in the interval $[-1, 1]$ which can also be determined explicitly.

In [KMcG] one finds an explicit expression for the Stieltjes transform of the measure in question, from which by use of the classical theory it follows that the absolutely continuous part of the measure is given by the density

$$\frac{\sqrt{4pq - x^2}}{(p - p_0)x^2 - r_0(2p - p_0)x + r_0^2 p + p_0^2 q}$$

supported in the interval $|x| \leqslant \sqrt{4pq}$. Depending on the values of p, p_0, r_0 one may have extra point masses in the orthogonality measure $\mathrm{d}\psi(x)$ introduced above.

In the case of a birth and death process it is, of course, useful to think of a graph like



The nodes here represent the states $0, 1, 2, \ldots$ and the arrows go along with the one step transition probabilities. One should imagine that the graph extends all the way to the right.

The ideas behind the Karlin–McGregor formula seen earlier can be used to study more complicated random walks. This is the point of the next section. All these developments are part of a very classical line of work that starts with the moment problem and its powerful connections with spectral theory. The reader will find lots of historical material along these lines in [A, DS, S]. For a nice recent presentation see [Si].

2. Going back to M G Krein

Given a positive definite matrix-valued smooth weight function $W(x)$ with finite moments, consider the skew symmetric bilinear form defined for any pair of matrix-valued polynomial functions $P(x)$ and $Q(x)$ by the numerical matrix

$$(P, Q) = (P, Q)_W = \int_{\mathbb{R}} P(x)W(x)Q^*(x)\mathrm{d}x,$$

where $Q^*(x)$ denotes the conjugate transpose of $Q(x)$.

By the usual Gram–Schmidt construction this leads to the existence of a sequence of matrix-valued orthogonal polynomials with non-singular leading coefficient, $P_n(x) = M_n x^n + M_{n-1}x^{n-1} + \cdots$.

Given an orthogonal sequence $\{P_n(x)\}_{n\geqslant 0}$ of matrix-valued orthogonal polynomials one gets by the usual argument a three term recursion relation

$$xP_n(x) = A_n P_{n-1}(x) + B_n P_n(x) + C_n P_{n+1}(x), \tag{1}$$

where A_n, B_n and C_n are matrices and the last one is non-singular. All of this is due to M G Krein (see [K1, K2]).

It is convenient to introduce the block tridiagonal matrix $\mathbb{P}$:

$$\mathbb{P} = \begin{pmatrix} B_0 & C_0 & & \\ A_1 & B_1 & C_1 & \\ & \ddots & \ddots & \ddots \end{pmatrix}.$$

If $\mathbb{P}_{i,j}$ denotes the i, j block of $\mathbb{P}$ we can generate a sequence of matrix-valued polynomials $Q_i(x)$ by imposing the three term recursion given above. Following the notation of the scalar case, we have

$$\mathbb{P}Q(x) = xQ(x),$$

where the entries of the column vector $Q(x)$ are now matrices.

Proceeding as in the scalar case, this relation can be iterated to give

$$\mathbb{P}^n Q(x) = x^n Q(x)$$

and if we assume the existence of a weight matrix $W(x)$ as in Krein's theory, with the property

$$(Q_j, Q_j)\delta_{i,j} = \int_{\mathbb{R}} Q_i(x)W(x)Q_j^*(x)\mathrm{d}x,$$

it is then clear that one can get an expression for the (i, j) entry of the block matrix $\mathbb{P}^n$ that would look exactly as in the scalar case, namely

$$(\mathbb{P}^n)_{ij}(Q_j, Q_j) = \int x^n Q_i(x)W(x)Q_j^*(x)\mathrm{d}x.$$

Just as in the scalar case, this expression becomes useful when we can get our hands on the matrix-valued polynomials $Q_i(x)$ and the orthogonality measure $W(x)$. This is the purpose of this paper in the case of a specific network to be described later on. Note that we have not discussed conditions on the matrix $\mathbb{P}$ to give rise to a measure as in the case originally considered by M G Krein, where he assumes that the matrices C_i and A_{i+1} in $\mathbb{P}$ are the adjoints of each other and that the matrices B_i are symmetric. One can show that the required condition is that the matrix $\mathbb{P}$ should be block-symmetrizable, i.e. by conjugating with a block-diagonal matrix $\mathbb{P}$ should become the type of matrix considered in [K1, K2]. This point has been addressed in theorem 2.1 of [DRSZ].

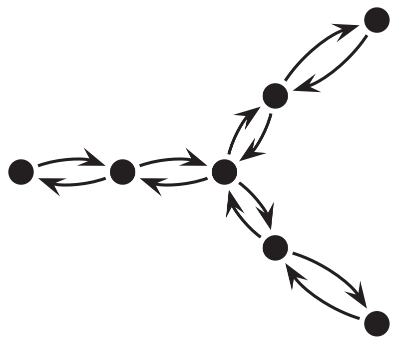
3. Spider graphs and its variant

In queueing theory people consider discrete time Markov chains where the state space is given by pairs of integers (n,i) with $n = 0, 1, 2, \ldots$ and i between 1 and a fixed m. The first coordinate is called the level and the second one the phase of the state (n, j). One is then led to consider a block tridiagonal matrix as the one-step transition probability of the Markov chain if transitions in one step are restricted to states in the same level or in the two adjacent levels. This is a natural area to look for useful applications of the theory of matrix-valued orthogonal polynomials. For a good reference to the queueing models, where these models are called *Quasi-birth-and-death process* (QBD) (see [BB, LR, N, LPT, DRSZ, G2]).

In [GdI], we manage to find the orthogonal (matrix-valued) polynomials, the orthogonality matrix-valued measure, and we find explicitly the invariant measure for the process in question. The reader should note that in the case of an ordinary birth-and-death process, such as in [KMcG] one can prove that the norms of the scalar polynomials $Q_j(x)$ give a way to produce an invariant measure. The point is that the ratio of two consecutive components of the invariant measure is given by the inverse of the ratio of the squares of the norms of the orthogonal polynomials. This is a well-known fact, and a simple proof is given in [GdI].

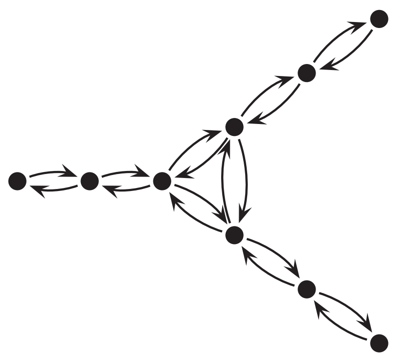
In the block tridiagonal case there is no guarantee that this trick will always work, since the matrix-valued polynomials $Q_j(x)$ will in general have matrix-valued norms. In the case considered in [GdI] the norms are diagonal matrices and give a good way to compute the invariant measure, just as in the scalar case. We will return to this point in the last section of this paper.

Another paper where a similar type of study is made is [DRSZ]. In this paper the authors study a number of previously known examples and they consider a new one, depicted by the network of the type given below, where each of the arms extends to infinity.



I have analyzed this network in [G3] and obtained an explicit expression for its spectral measure. It is not obvious how to make such a network into one that can be analyzed by means of matrix-valued orthogonal polynomials, but this can be done, as shown nicely in [DRSZ], and in this fashion one can start analyzing many complicated direct as well as inverse problems for large classes of networks. For some extra details see [DRSZ] and the next section in this paper.

In this paper I consider a variant of the spider graph depicted above, namely one that looks as in the graph below, where once again the external arms extend to infinity.



4. Some analytical results

Here we collect a few analytical results which are useful in determining the orthogonality weight for the matrix orthogonal polynomials that go with a block tridiagonal matrix such as the one given in section 2.

The results below are very useful already in the case when one is dealing with ordinary tridiagonal matrices and the corresponding scalar-valued orthogonal polynomials, and they were used in [KMcG] to obtain—in the scalar valued case—the orthogonality weight of some random walks starting from simpler ones. We will use the same method in the matrix-valued case.

It is hard to trace the history of these well-known results accurately, but certainly the main contributors include people like T Stieltjes and A Markov. For a guide to the literature see [DS, S, Si].

Denote by $\mathbb{P}$ the block-tridiagonal matrix

$$\mathbb{P} = \begin{pmatrix} B_0 & C_0 & & & \\ A_1 & B_1 & C_1 & & \\ & A_2 & B_2 & C_2 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

and by $\tilde{\mathbb{P}}$ the matrix obtained from $\mathbb{P}$ by erasing the first row and column of block matrices.

Let $\mathrm{d}\Sigma(x)$ and $\mathrm{d}\tilde{\Sigma}(x)$ denote the matrix-valued measures that give

$$\mathbb{P} = \int x \mathrm{d}\Sigma(x)$$

and

$$\tilde{\mathbb{P}} = \int x \mathrm{d}\tilde{\Sigma}(x).$$

Introduce the matrix-valued function given by

$$\Theta(x) = \int \frac{\mathrm{d}\Sigma(x)}{1 - xz} = \sum_{n=0}^{\infty} S_n z^n$$

with

$$S_n = \int x^n \mathrm{d}\Sigma(x).$$

If we denote with $\tilde{\Theta}(z)$, $\tilde{S}_n$ the corresponding objects for the matrix $\tilde{\mathbb{P}}$, then it is not hard to see that

$$\Theta(z) S_0^{-1}\left(I - zB_0 - z^2 C_0 \tilde{\Theta}(z) \tilde{S}_0^{-1} A_1\right) = I.$$

In terms of the Stieltjes transforms

$$B(z) = \int \frac{\mathrm{d}\Sigma(x)}{x - z}$$

and

$$\tilde{B}(z) = \int \frac{\mathrm{d}\tilde{\Sigma}(x)}{x - z}$$

one can rewrite the identity above in the form

$$B(z) S_0^{-1}\left(z - B_0 + C_0 \tilde{B}(z) \tilde{S}_0^{-1} A_1\right) + I = 0.$$

Formulae of this type appear in [AN] and a nice and simple proof is indicated in [DPS] and credited to I. Schur. It is clear that the use of Schur complements can be used to great advantage when in dealing with matrix-valued orthogonal polynomials. One can find expressions related to these ones in theorem 2.6 of [DRSZ]. In that case some of the proofs are based on results in [D1, D2].

To obtain $\mathrm{d}\Sigma$ form $\tilde{\mathrm{d}}\Sigma$ one still needs to recall what is usually called the Stieltjes inversion formula which recovers a measure form its Stieltjes transform. For a good reference the reader may want to consult [Wa].

We will use this method to compute the orthogonality measure going with the 'spider graph' as well as its variant indicated in the picture above and explained in detail in the next section.

In the case of the 'spider graph' the result has already been given in [G3] where the result was obtained by more painful methods. The use of what we call the Stieltjes method gives a more compact form for the continuous part of the measure. As indicated in [G3] if $p > 1/2$ the measure coincides with its continuous part. For $p < 1/2$ one needs to add delta masses (with matrix valued coefficients) at the points -1 and 1.

For the 'spider graph' with N legs, first considered in [DRSZ], in the notation of section 2 we have

$$B_0 = \begin{pmatrix} 0 & x_2 & x_3 & \dots & x_N \\ q & 0 & 0 & & 0 \\ q & & & & \\ \vdots & & & & \\ q & & & & \end{pmatrix}$$

$$C_0 = \begin{pmatrix} x_1 & 0 & 0 & \dots & 0 \\ 0 & p & & & \\ & & p & & \\ & & & \ddots & \\ 0 & 0 & 0 & \dots & p \end{pmatrix}$$

and

$$C_i \equiv pI, \qquad i \geqslant 1; B_i = 0I, \qquad i \geqslant 1; A_i = qI, \qquad i \geqslant 1.$$

Consider now the symmetrized version of this matrix and the polynomials that come about by choosing the first polynomial $P_0(x)$ as the diagonal matrix with entries

$$1, \sqrt{x_{N-1}/q}, \sqrt{x_{N-2}/q}, \dots, \sqrt{x_1/q}.$$

The use of the Stieltjes inversion method and the rest of the strategy described above give for the continuous part of the matrix-valued orthogonality weight a simple expression. The support of the measure is the interval $|x| \leqslant \sqrt{4pq}$, and the measure consists of a scalar factor, namely

$$\frac{\sqrt{4pq - x^2}}{1 - x^2},$$

multiplied by a quadratic polynomial in x with $N \times N$ matrix coefficients given as follows:

Consider a matrix whose elements in the first row and column equal to zero, except the $1, 1$ element which is p/q. Of the remaining elements the diagonal ones are given by $(1 - x_i)/x_{N-j+1}$ and the off-diagonal ones by $-\sqrt{x_i x_j/(x_{N-i+1}x_{N-j+1})}$. This matrix is then multiplied by the factor q/p and this gives the constant term.

The coefficient of degree 1 in x is a symmetric matrix where all elements vanish except for the first row starting with the entry $1, 2$ and going to the right. The $1, j$ entry is $\sqrt{x_j/x_{N-j+1}}$. The symmetric nature of this matrix dictates the elements of the first column.

Consider a matrix with the first row and column identically zero. The remaining elements have the values $(x_i - q)/x_{N-j+1}$ on the main diagonal and the off-diagonal ones are given by $\sqrt{x_i x_j/(x_{N-i+1}x_{N-j+1})}$. This matrix is multiplied by $1/p$ to give the coefficient of the quadratic term in x.

5. A variant of a spider graph

For concreteness we will treat in detail the case of the graph given at the end of section 3 but we write below the matrices that are used to generate the orthogonal polynomials in the case of N legs going to infinity.

One has a center core and N legs that extend to infinity. If drawn properly the nodes on these legs form a sequence of concentric circles surrounding the central core. This is clearly a variant of a discrete version of the spiders considered by J B Walsh, [W, ES].

It is convenient to label the nodes in the center core as $1, 2, \ldots N$ and then the N nodes on the first circle as $N+1, N+2, \ldots, 2N$ in a counter-clockwise fashion. The N nodes in the second circle are labeled as $2N+1, 2N+2, \ldots, 3N$, etc. The transition probabilities from each of the nodes in the center core to each one of the remaining $N-1$ nodes on the core are taken to be $\frac{1-p}{N-1}$. The transition probability from each one of these nodes in the core to the one node on the corresponding leg and located on the first circle is p.

For each node that is not on the center core, and therefore lies on one of the legs of the graph, the probability of getting closer to the center core, while remaining on the same leg, is given by the common value $q = 1-p$ while the probability of a transition moving one step away from the center core, while staying on the same leg, is given by the common value p.

It is now convenient to consider $N \times N$ matrix-valued orthogonal polynomials $Q_j(x)$ resulting from a block tridiagonal matrix with blocks given by the following expressions

$$B_0 = \begin{pmatrix} 0 & (1-p)/(N-1) & (1-p)/(N-1) & \ldots & (1-p)/(N-1) \\ (1-p)/(N-1) & 0 & (1-p)/(N-1) & \ldots & (1-p)/(N-1) \\ (1-p)/(N-1) & & & & \\ \vdots & & & & \\ (1-p)/(N-1) & (1-p)/(N-1) & (1-p)/(N-1) & \ldots & 0 \end{pmatrix}$$

and

$$A_i \equiv qI, \qquad i \geqslant 1; \; B_i \equiv 0I, \qquad i \geqslant 1; \; C_i \equiv pI, \qquad i \geqslant 0.$$

We move now to the task of finding a 3×3 matrix-valued weight that makes the corresponding polynomials, obtained from the recursion relation mentioned at the beginning of the paper, orthogonal. Just as in the case of the 'spider graph' considered in the previous section, one can use the Stieltjes method.

The orthogonality matrix consists of up to three parts. There is always an absolutely continuous matrix-valued density supported in the interval $|x| \leqslant \sqrt{4pq}$, and given by

$$\frac{\sqrt{4pq - x^2}}{2(1-x)(p-1)(2x+3p+1)} \begin{pmatrix} \alpha(x) & \beta(x) & \beta(x) \\ \beta(x) & \alpha(x) & \beta(x) \\ \beta(x) & \beta(x) & \alpha(x) \end{pmatrix}$$

with

$$\alpha(x) = 2x - p - 3; \qquad \beta(x) = -(2x + p - 1).$$

In the case when $1/5 < p < 1/2$ we need to add a discrete matrix-valued mass

$$\frac{1-2p}{3(1-p)}\pi \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \delta_1.$$

In the case when $p < 1/5$ there is one more piece to be included in the weight matrix, namely,

$$\frac{(1-5p)}{3(1-p)}\pi \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \delta_{x_p},$$

where

$$x_p = -1/2 - 3p/2.$$

The point x_p is always outside of the support of the density, and thus both delta masses (when present) have supports outside the support of the density.

It is easy to write the orthogonal polynomials $Q_j(x)$ themselves in terms of the simpler polynomials $T_j(x)$ (which one may want to refer to as the Chebyshev polynomials) corresponding to the same choice of matrix-valued coefficients as above, with the exception of the matrix B_0 which is now set equal to the zero matrix. If these simpler polynomials are denoted by $T_j(x)$ we get for our polynomials $Q_j(x)$ the expression

$$Q_j(x) = T_j(x) + \frac{p-1}{2p} T_{j-1}(x) \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

6. The invariant measure

Given any Markov chain the explicit computation of an invariant measure is a non-trivial task. In the case of a birth-and-death process we recalled in section 3 that the norms of the orthogonal polynomials give an expression for the invariant measure. This method is not guaranteed to work, as we remarked earlier, for an arbitrary Markov chain obtained from a block tridiagonal matrix. However in the case at hand, we get lucky, since the matrix-valued squared norms of the successive polynomials $Q_i(x)$ given above happen to be diagonal and given by

$$\|Q_i\|^2 = (q/p)^i \pi I.$$

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